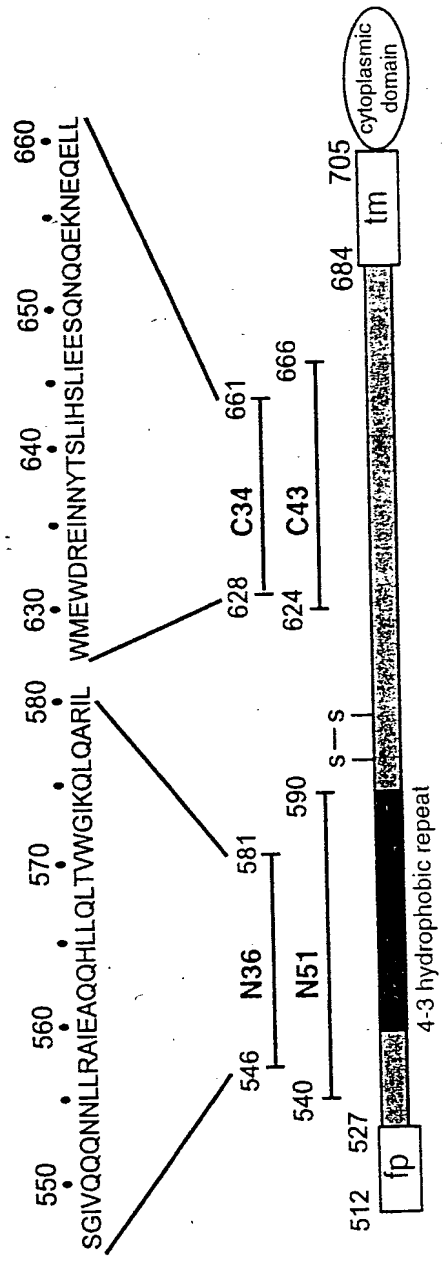
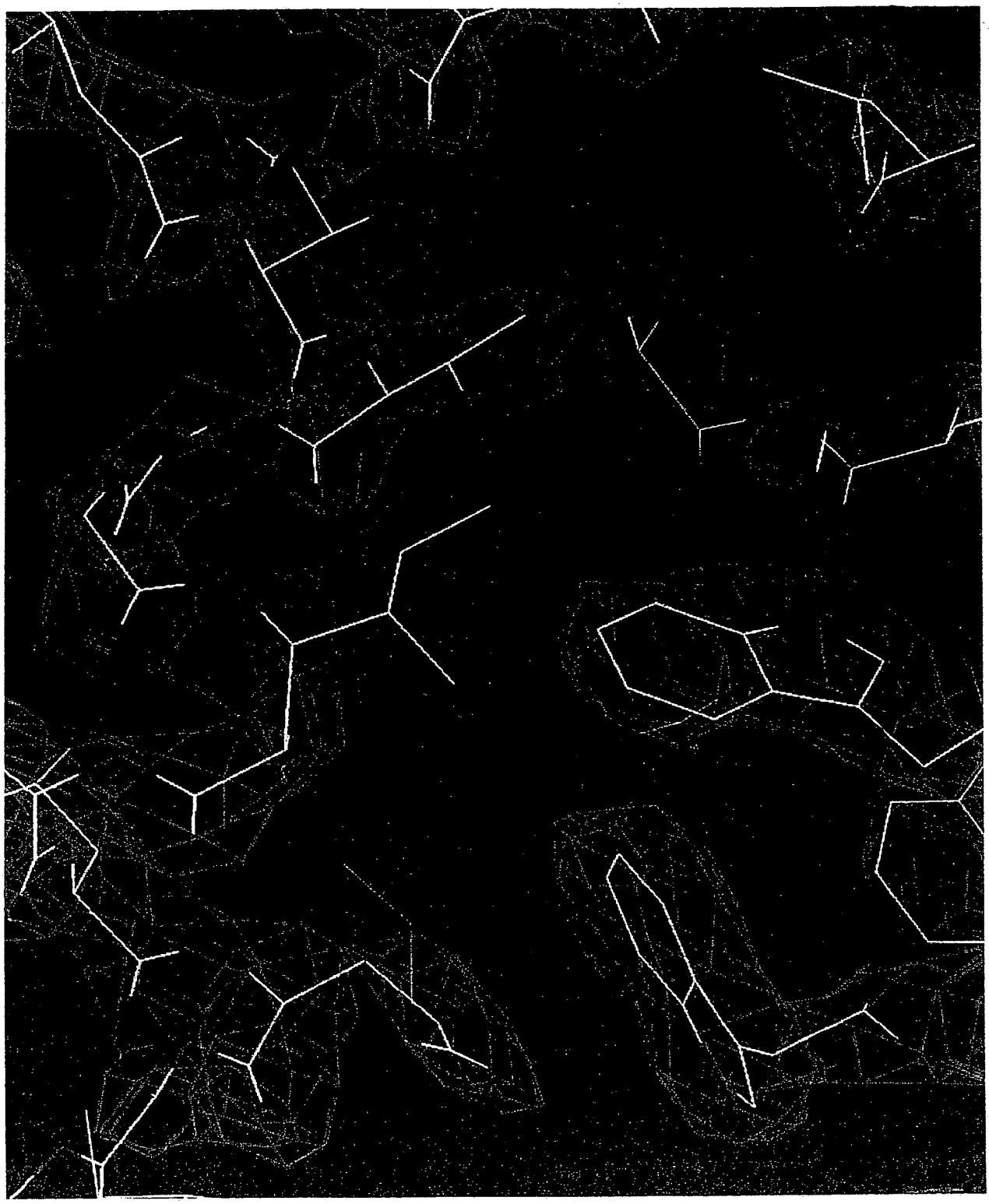


FIG. 1

BEST AVAILABLE COPY

FIG. 2



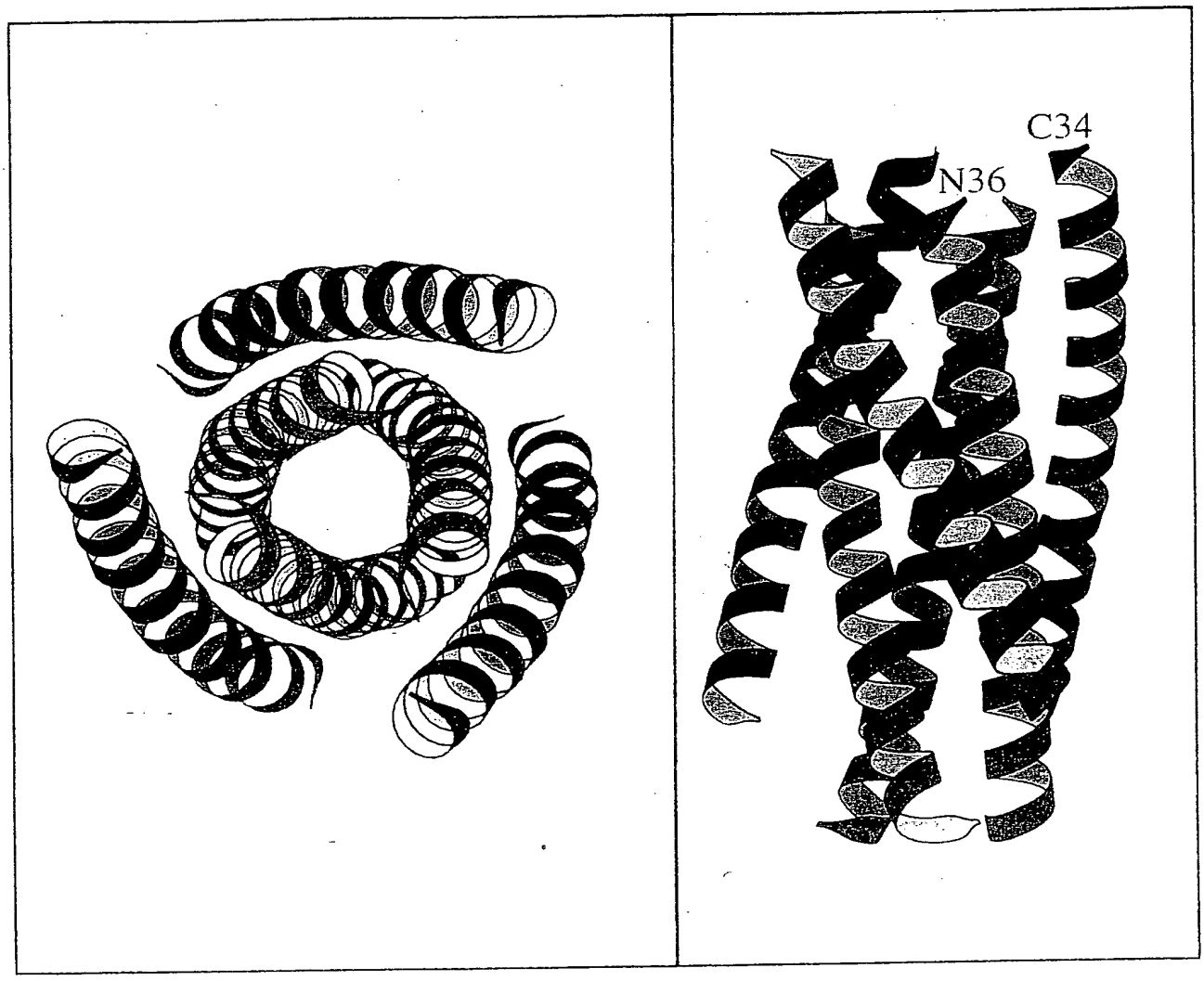
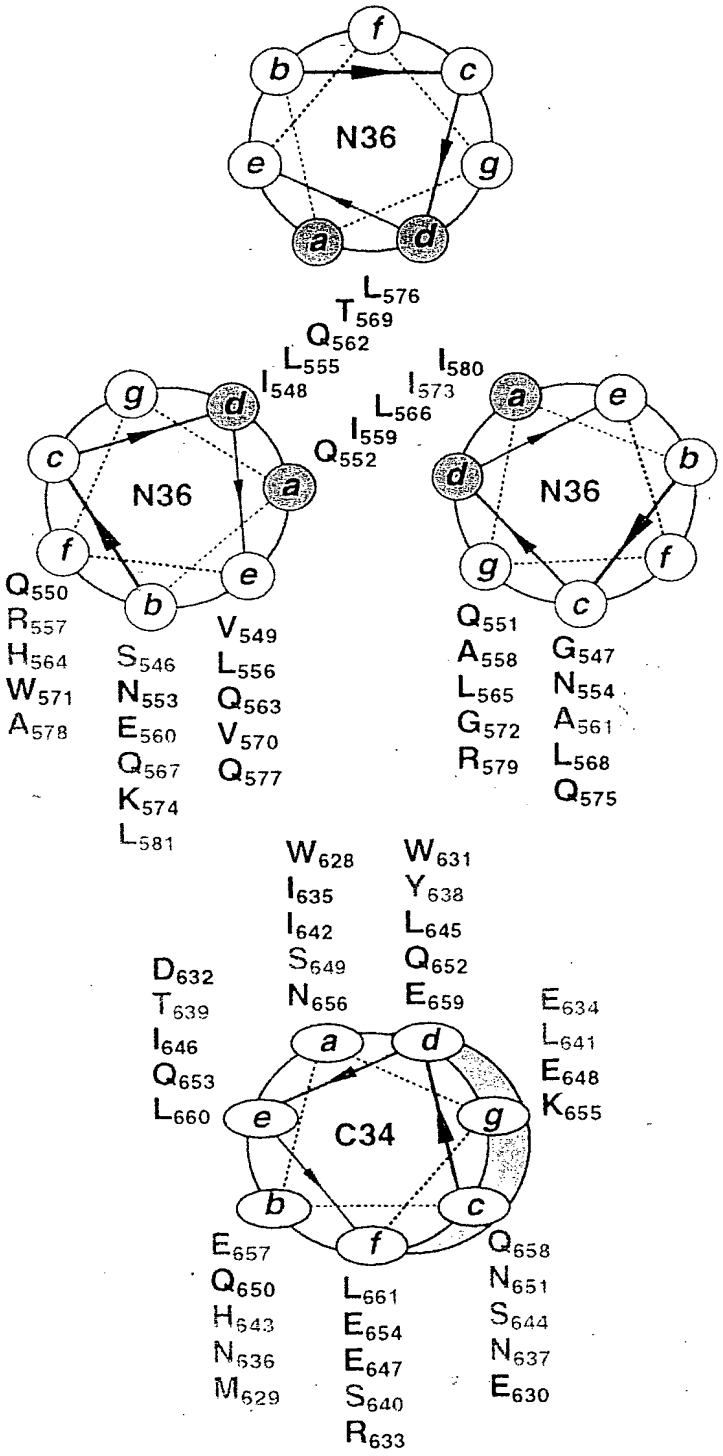


FIG. 3A

FIG. 3B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N36
N36
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T569
Q562
L555
I548
I580
I573
L566
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Q552
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R557
H564
W571
A578
S546
N553
E560
Q567
K574
L581
V549
L556
Q563
V570
Q577
Q551
A558
L565
G572
R579
G547
N554
A561
L568
Q575
W628
I635
I642
S649
N656
W631
Y638
L645
Q652
E659
D632
T639
I646
Q653
L660
E634
L641
E648
K655
E657
Q650
H643
N636
M629
L661
E654
E647
S640
R633
Q658
N651
S644
N637
E630

FIG. 4

```
CRYST1   49.500   49.500   55.300  90.00  90.00 120.00 P 3 2 1          6
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.020202  0.011664  0.000000        0.00000
SCALE2      0.000000  0.023327  0.000000        0.00000
SCALE3      0.000000  0.000000  0.018083        0.00000
HETATM    1  C   ACE N   0      19.211  14.270 -17.472  1.00 56.26           C
HETATM    2  O   ACE N   0      19.488  14.580 -16.305  1.00 56.37           O
HETATM    3  CH3 ACE N   0      20.273  14.045 -18.531  1.00 56.01           C
ATOM      4  N   SER N 546      17.955  14.014 -17.827  1.00 56.49           N
ATOM      5  CA  SER N 546      16.876  14.392 -16.942  1.00 56.15           C
ATOM      6  C   SER N 546      16.909  13.631 -15.655  1.00 56.24           C
ATOM      7  O   SER N 546      16.736  14.255 -14.615  1.00 57.67           O
ATOM      8  CB  SER N 546      15.525  14.172 -17.546  1.00 56.05           C
ATOM      9  OG  SER N 546      15.498  12.815 -17.842  1.00 57.84           O
ATOM     10  H   SER N 546      17.816  13.501 -18.652  1.00  0.00           H
ATOM     11  HG  SER N 546      15.988  12.455 -18.582  1.00  0.00           H
ATOM     12  N   GLY N 547      17.181  12.316 -15.724  1.00 55.59           N
ATOM     13  CA  GLY N 547      17.202  11.414 -14.570  1.00 53.04           C
ATOM     14  C   GLY N 547      18.299  11.783 -13.596  1.00 51.70           C
ATOM     15  O   GLY N 547      18.147  11.667 -12.391  1.00 50.76           O
ATOM     16  H   GLY N 547      17.409  11.945 -16.618  1.00  0.00           H
ATOM     17  N   ILE N 548      19.399  12.280 -14.145  1.00 51.57           N
ATOM     18  CA  ILE N 548      20.551  12.815 -13.425  1.00 52.14           C
ATOM     19  C   ILE N 548      20.218  14.116 -12.696  1.00 51.31           C
ATOM     20  O   ILE N 548      20.543  14.273 -11.519  1.00 50.83           O
ATOM     21  CB  ILE N 548      21.693  13.043 -14.436  1.00 54.22           C
ATOM     22  CG1 ILE N 548      22.120  11.712 -15.087  1.00 54.58           C
ATOM     23  CG2 ILE N 548      22.861  13.705 -13.721  1.00 55.25           C
ATOM     24  CD1 ILE N 548      23.126  11.909 -16.234  1.00 56.29           C
ATOM     25  H   ILE N 548      19.445  12.272 -15.118  1.00  0.00           H
ATOM     26  N   VAL N 549      19.590  15.054 -13.393  1.00 50.93           N
ATOM     27  CA  VAL N 549      19.093  16.291 -12.786  1.00 50.79           C
ATOM     28  C   VAL N 549      18.036  15.977 -11.726  1.00 50.36           C
ATOM     29  O   VAL N 549      17.992  16.598 -10.674  1.00 51.60           O
ATOM     30  CB  VAL N 549      18.451  17.196 -13.841  1.00 52.28           C
ATOM     31  CG1 VAL N 549      17.814  18.437 -13.226  1.00 54.97           C
ATOM     32  CG2 VAL N 549      19.539  17.650 -14.780  1.00 51.05           C
ATOM     33  H   VAL N 549      19.486  14.911 -14.360  1.00  0.00           H
ATOM     34  N   GLN N 550      17.187  15.030 -12.001  1.00 49.13           N
ATOM     35  CA  GLN N 550      16.176  14.508 -11.109  1.00 49.23           C
ATOM     36  C   GLN N 550      16.843  13.895  -9.861  1.00 48.50           C
ATOM     37  O   GLN N 550      16.520  14.236  -8.736  1.00 47.94           O
ATOM     38  CB  GLN N 550      15.452  13.398 -11.814  1.00 52.96           C
ATOM     39  CG  GLN N 550      13.929  13.475 -11.925  1.00 60.75           C
ATOM     40  CD  GLN N 550      13.343  13.742 -10.585  1.00 65.31           C
ATOM     41  OE1 GLN N 550      13.048  14.884 -10.294  1.00 71.73           O
ATOM     42  NE2 GLN N 550      13.111  12.750  -9.753  1.00 67.42           N
ATOM     43  H   GLN N 550      17.256  14.628 -12.913  1.00  0.00           H
ATOM     44 1HE2 GLN N 550      12.689  12.960  -8.892  1.00  0.00           H
ATOM     45 2HE2 GLN N 550      13.298  11.810 -10.020  1.00  0.00           H
ATOM     46  N   GLN N 551      17.847  13.009 -10.014  1.00 47.87           N
ATOM     47  CA  GLN N 551      18.607  12.368  -8.940  1.00 47.02           C
ATOM     48  C   GLN N 551      19.320  13.416  -8.092  1.00 45.81           C
ATOM     49  O   GLN N 551      19.330  13.334  -6.868  1.00 46.09           O
ATOM     50  CB  GLN N 551      19.605  11.378  -9.582  1.00 45.66           C
ATOM     51  CG  GLN N 551      20.600  10.535  -8.719  1.00 41.50           C
```

FIG. 5A

```
ATOM     52  CD  GLN N 551      19.994   9.589  -7.719  1.00 39.83           C
ATOM     53  OE1 GLN N 551      18.955   9.872  -7.134  1.00 42.03           O
ATOM     54  NE2 GLN N 551      20.573   8.430  -7.469  1.00 34.15           N
ATOM     55  H   GLN N 551      18.103  12.786 -10.928  1.00  0.00           H
ATOM     56 1HE2 GLN N 551      20.183   7.817  -6.808  1.00  0.00           H
ATOM     57 2HE2 GLN N 551      21.382   8.205  -7.988  1.00  0.00           H
ATOM     58  N   GLN N 552      19.874  14.445  -8.725  1.00 45.32           N
ATOM     59  CA  GLN N 552      20.538  15.562  -8.041  1.00 44.72           C
ATOM     60  C   GLN N 552      19.620  16.316  -7.096  1.00 43.57           C
ATOM     61  O   GLN N 552      19.987  16.732  -6.006  1.00 41.76           O
ATOM     62  CB  GLN N 552      21.115  16.542  -9.078  1.00 46.04           C
ATOM     63  CG  GLN N 552      22.500  16.015  -9.433  1.00 50.92           C
ATOM     64  CD  GLN N 552      23.257  16.787 -10.486  1.00 54.67           C
ATOM     65  OE1 GLN N 552      22.658  17.525 -11.260  1.00 59.31           O
ATOM     66  NE2 GLN N 552      24.575  16.670 -10.575  1.00 56.36           N
ATOM     67  H   GLN N 552      19.818  14.442  -9.707  1.00  0.00           H
ATOM     68 1HE2 GLN N 552      24.996  17.210 -11.277  1.00  0.00           H
ATOM     69 2HE2 GLN N 552      25.079  16.087  -9.993  1.00  0.00           H
ATOM     70  N   ASN N 553      18.383  16.452  -7.534  1.00 43.26           N
ATOM     71  CA  ASN N 553      17.350  17.053  -6.728  1.00 43.57           C
ATOM     72  C   ASN N 553      17.047  16.173  -5.554  1.00 42.82           C
ATOM     73  O   ASN N 553      16.914  16.649  -4.433  1.00 43.18           O
ATOM     74  CB  ASN N 553      16.050  17.238  -7.509  1.00 46.51           C
ATOM     75  CG  ASN N 553      15.095  18.168  -6.802  1.00 51.48           C
ATOM     76  OD1 ASN N 553      15.256  18.608  -5.669  1.00 59.01           O
ATOM     77  ND2 ASN N 553      14.006  18.540  -7.412  1.00 57.62           N
ATOM     78  H   ASN N 553      18.168  16.200  -8.470  1.00  0.00           H
ATOM     79 1HD2 ASN N 553      13.333  19.036  -6.902  1.00  0.00           H
ATOM     80 2HD2 ASN N 553      13.822  18.181  -8.313  1.00  0.00           H
ATOM     81  N   ASN N 554      17.005  14.883  -5.807  1.00 42.25           N
ATOM     82  CA  ASN N 554      16.731  13.930  -4.736  1.00 43.15           C
ATOM     83  C   ASN N 554      17.876  13.908  -3.715  1.00 42.63           C
ATOM     84  O   ASN N 554      17.628  13.893  -2.508  1.00 42.65           O
ATOM     85  CB  ASN N 554      16.534  12.538  -5.331  1.00 44.49           C
ATOM     86  CG  ASN N 554      15.340  12.520  -6.239  1.00 48.97           C
ATOM     87  OD1 ASN N 554      14.277  13.033  -5.925  1.00 51.91           O
ATOM     88  ND2 ASN N 554      15.485  12.022  -7.460  1.00 52.70           N
ATOM     89  H   ASN N 554      17.137  14.573  -6.736  1.00  0.00           H
ATOM     90 1HD2 ASN N 554      14.691  11.924  -8.059  1.00  0.00           H
ATOM     91 2HD2 ASN N 554      16.321  11.585  -7.671  1.00  0.00           H
ATOM     92  N   LEU N 555      19.125  14.034  -4.177  1.00 41.19           N
ATOM     93  CA  LEU N 555      20.270  14.065  -3.310  1.00 39.88           C
ATOM     94  C   LEU N 555      20.274  15.341  -2.498  1.00 40.16           C
ATOM     95  O   LEU N 555      20.383  15.280  -1.272  1.00 40.42           O
ATOM     96  CB  LEU N 555      21.556  13.984  -4.115  1.00 37.85           C
ATOM     97  CG  LEU N 555      21.762  12.724  -4.945  1.00 38.85           C
ATOM     98  CD1 LEU N 555      23.106  12.783  -5.687  1.00 39.10           C
ATOM     99  CD2 LEU N 555      21.643  11.526  -4.019  1.00 36.44           C
ATOM    100  H   LEU N 555      19.245  14.101  -5.145  1.00  0.00           H
ATOM    101  N   LEU N 556      20.097  16.504  -3.139  1.00 39.83           N
ATOM    102  CA  LEU N 556      20.056  17.800  -2.490  1.00 39.00           C
ATOM    103  C   LEU N 556      18.997  17.825  -1.428  1.00 40.28           C
ATOM    104  O   LEU N 556      19.251  18.290  -0.326  1.00 40.24           O
ATOM    105  CB  LEU N 556      19.769  18.896  -3.504  1.00 37.52           C
ATOM    106  CG  LEU N 556      19.826  20.327  -2.982  1.00 35.51           C
ATOM    107  CD1 LEU N 556      21.227  20.634  -2.595  1.00 38.30           C
ATOM    108  CD2 LEU N 556      19.383  21.304  -4.051  1.00 35.56           C
ATOM    109  H   LEU N 556      20.042  16.470  -4.118  1.00  0.00           H
```

FIG. 5B

```
ATOM    110  N   ARG N 557      17.823  17.292  -1.689  1.00 41.01           N
ATOM    111  CA  ARG N 557      16.776  17.288  -0.685  1.00 42.31           C
ATOM    112  C   ARG N 557      17.200  16.394   0.467  1.00 42.26           C
ATOM    113  O   ARG N 557      17.012  16.740   1.622  1.00 42.69           O
ATOM    114  CB  ARG N 557      15.457  16.809  -1.356  1.00 45.42           C
ATOM    115  CG  ARG N 557      14.746  17.951  -2.111  1.00 50.30           C
ATOM    116  CD  ARG N 557      13.344  17.553  -2.601  1.00 57.56           C
ATOM    117  NE  ARG N 557      13.280  16.625  -3.751  1.00 64.22           N
ATOM    118  CZ  ARG N 557      12.355  15.631  -3.918  1.00 63.91           C
ATOM    119  NH1 ARG N 557      11.397  15.396  -3.011  1.00 64.47           N
ATOM    120  NH2 ARG N 557      12.335  14.867  -5.036  1.00 59.98           N
ATOM    121  H   ARG N 557      17.638  16.953  -2.607  1.00  0.00           H
ATOM    122  HE  ARG N 557      13.950  16.746  -4.463  1.00  0.00           H
ATOM    123 1HH1 ARG N 557      11.350  15.933  -2.167  1.00  0.00           H
ATOM    124 2HH1 ARG N 557      10.752  14.634  -3.142  1.00  0.00           H
ATOM    125 1HH2 ARG N 557      12.994  15.016  -5.779  1.00  0.00           H
ATOM    126 2HH2 ARG N 557      11.659  14.126  -5.135  1.00  0.00           H
ATOM    127  N   ALA N 558      17.915  15.313   0.192  1.00 41.57           N
ATOM    128  CA  ALA N 558      18.387  14.409   1.226  1.00 41.10           C
ATOM    129  C   ALA N 558      19.392  15.061   2.144  1.00 40.54           C
ATOM    130  O   ALA N 558      19.295  14.930   3.360  1.00 39.05           O
ATOM    131  CB  ALA N 558      19.030  13.199   0.587  1.00 41.90           C
ATOM    132  H   ALA N 558      18.173  15.144  -0.746  1.00  0.00           H
ATOM    133  N   ILE N 559      20.294  15.861   1.569  1.00 41.09           N
ATOM    134  CA  ILE N 559      21.309  16.634   2.316  1.00 40.49           C
ATOM    135  C   ILE N 559      20.614  17.708   3.169  1.00 41.59           C
ATOM    136  O   ILE N 559      20.961  17.946   4.334  1.00 41.89           O
ATOM    137  CB  ILE N 559      22.333  17.310   1.315  1.00 37.40           C
ATOM    138  CG1 ILE N 559      23.112  16.223   0.558  1.00 35.03           C
ATOM    139  CG2 ILE N 559      23.294  18.213   2.061  1.00 36.22           C
ATOM    140  CD1 ILE N 559      23.944  16.723  -0.634  1.00 29.22           C
ATOM    141  H   ILE N 559      20.262  15.968   0.586  1.00  0.00           H
ATOM    142  N   GLU N 560      19.595  18.377   2.634  1.00 41.05           N
ATOM    143  CA  GLU N 560      18.927  19.411   3.378  1.00 41.53           C
ATOM    144  C   GLU N 560      18.194  18.774   4.529  1.00 41.42           C
ATOM    145  O   GLU N 560      18.199  19.290   5.659  1.00 42.58           O
ATOM    146  CB  GLU N 560      17.950  20.139   2.504 -1.00 42.94           C
ATOM    147  CG  GLU N 560      18.559  20.916   1.342  1.00 49.98           C
ATOM    148  CD  GLU N 560      17.569  21.635   0.403  1.00 56.47           C
ATOM    149  OE1 GLU N 560      16.353  21.580   0.624  1.00 58.21           O
ATOM    150  OE2 GLU N 560      18.018  22.257  -0.566  1.00 56.22           O
ATOM    151  H   GLU N 560      19.338  18.191   1.696  1.00  0.00           H
ATOM    152  N   ALA N 561      17.605  17.606   4.311  1.00 41.55           N
ATOM    153  CA  ALA N 561      16.886  16.905   5.362  1.00 41.77           C
ATOM    154  C   ALA N 561      17.880  16.505   6.441  1.00 42.70           C
ATOM    155  O   ALA N 561      17.661  16.726   7.641  1.00 42.40           O
ATOM    156  CB  ALA N 561      16.221  15.671   4.797  1.00 39.29           C
ATOM    157  H   ALA N 561      17.617  17.230   3.403  1.00  0.00           H
ATOM    158  N   GLN N 562      19.053  16.076   6.014  1.00 43.26           N
ATOM    159  CA  GLN N 562      20.042  15.666   6.986  1.00 43.97           C
ATOM    160  C   GLN N 562      20.607  16.819   7.771  1.00 43.53           C
ATOM    161  O   GLN N 562      20.989  16.658   8.934  1.00 43.63           O
ATOM    162  CB  GLN N 562      21.194  14.960   6.319  1.00 45.81           C
ATOM    163  CG  GLN N 562      20.703  13.620   5.857  1.00 48.45           C
ATOM    164  CD  GLN N 562      21.844  12.875   5.276  1.00 52.27           C
ATOM    165  OE1 GLN N 562      22.693  13.426   4.578  1.00 54.50           O
ATOM    166  NE2 GLN N 562      21.828  11.590   5.556  1.00 54.42           N
ATOM    167  H   GLN N 562      19.263  16.023   5.043  1.00  0.00           H
```

FIG. 5C

```
ATOM    168 1HE2 GLN N 562      22.558  11.067   5.175  1.00  0.00           H
ATOM    169 2HE2 GLN N 562      21.094  11.248   6.104  1.00  0.00           H
ATOM    170  N   GLN N 563      20.651  17.976   7.121  1.00 42.95           N
ATOM    171  CA  GLN N 563      21.100  19.166   7.761  1.00 43.75           C
ATOM    172  C   GLN N 563      20.156  19.484   8.886  1.00 44.90           C
ATOM    173  O   GLN N 563      20.607  19.846   9.965  1.00 45.57           O
ATOM    174  CB  GLN N 563      21.149  20.323   6.777  1.00 41.93           C
ATOM    175  CG  GLN N 563      21.818  21.547   7.400  1.00 41.15           C
ATOM    176  CD  GLN N 563      23.189  21.261   8.013  1.00 42.08           C
ATOM    177  OE1 GLN N 563      23.917  20.363   7.583  1.00 48.51           O
ATOM    178  NE2 GLN N 563      23.627  21.967   9.043  1.00 39.35           N
ATOM    179  H   GLN N 563      20.474  17.971   6.162  1.00  0.00           H
ATOM    180 1HE2 GLN N 563      24.526  21.732   9.369  1.00  0.00           H
ATOM    181 2HE2 GLN N 563      23.085  22.653   9.451  1.00  0.00           H
ATOM    182  N   HIS N 564      18.842  19.364   8.714  1.00 46.08           N
ATOM    183  CA  HIS N 564      17.909  19.582   9.830  1.00 47.34           C
ATOM    184  C   HIS N 564      18.133  18.647  10.985  1.00 46.35           C
ATOM    185  O   HIS N 564      18.167  19.105  12.118  1.00 45.28           O
ATOM    186  CB  HIS N 564      16.508  19.405   9.372  1.00 52.29           C
ATOM    187  CG  HIS N 564      16.122  20.497   8.389  1.00 58.12           C
ATOM    188  ND1 HIS N 564      15.024  20.554   7.683  1.00 63.16           N
ATOM    189  CD2 HIS N 564      16.858  21.617   8.051  1.00 61.99           C
ATOM    190  CE1 HIS N 564      15.029  21.609   6.945  1.00 62.90           C
ATOM    191  NE2 HIS N 564      16.140  22.240   7.177  1.00 62.40           N
ATOM    192  H   HIS N 564      18.535  19.251   7.783  1.00  0.00           H
ATOM    193  HD1 HIS N 564      14.318  19.929   7.750  1.00  0.00           H
ATOM    194  HE2 HIS N 564      16.408  23.027   6.657  1.00  0.00           H
ATOM    195  N   LEU N 565      18.352  17.382  10.651  1.00 46.30           N
ATOM    196  CA  LEU N 565      18.728  16.389  11.627  1.00 47.50           C
ATOM    197  C   LEU N 565      20.023  16.771  12.360  1.00 47.96           C
ATOM    198  O   LEU N 565      20.106  16.694  13.603  1.00 47.27           O
ATOM    199  CB  LEU N 565      18.955  15.028  10.980  1.00 48.98           C
ATOM    200  CG  LEU N 565      17.893  13.938  10.810  1.00 50.24           C
ATOM    201  CD1 LEU N 565      18.612  12.580  10.876  1.00 49.28           C
ATOM    202  CD2 LEU N 565      16.843  13.988  11.920  1.00 52.14           C
ATOM    203  H   LEU N 565      18.325  17.139   9.702  1.00  0.00           H
ATOM    204  N   LEU N 566      21.033  17.256  11.622  1.00 47.51           N
ATOM    205  CA  LEU N 566      22.278  17.716  12.229  1.00 48.90           C
ATOM    206  C   LEU N 566      22.041  18.835  13.232  1.00 48.39           C
ATOM    207  O   LEU N 566      22.563  18.779  14.346  1.00 47.61           O
ATOM    208  CB  LEU N 566      23.299  18.205  11.144  1.00 50.19           C
ATOM    209  CG  LEU N 566      24.223  17.163  10.521  1.00 50.83           C
ATOM    210  CD1 LEU N 566      24.767  17.627   9.151  1.00 45.72           C
ATOM    211  CD2 LEU N 566      25.295  16.848  11.579  1.00 50.85           C
ATOM    212  H   LEU N 566      20.921  17.339  10.656  1.00  0.00           H
ATOM    213  N   GLN N 567      21.182  19.797  12.902  1.00 48.03           N
ATOM    214  CA  GLN N 567      20.839  20.897  13.794  1.00 48.69           C
ATOM    215  C   GLN N 567      20.124  20.425  15.041  1.00 48.44           C
ATOM    216  O   GLN N 567      20.379  20.878  16.165  1.00 48.89           O
ATOM    217  CB  GLN N 567      19.940  21.927  13.071  1.00 49.47           C
ATOM    218  CG  GLN N 567      20.632  22.647  11.906  1.00 56.49           C
ATOM    219  CD  GLN N 567      21.964  23.290  12.278  1.00 63.24           C
ATOM    220  OE1 GLN N 567      22.393  23.265  13.426  1.00 66.99           O
ATOM    221  NE2 GLN N 567      22.723  23.924  11.394  1.00 68.66           N
ATOM    222  H   GLN N 567      20.769  19.768  12.006  1.00  0.00           H
ATOM    223 1HE2 GLN N 567      23.539  24.303  11.833  1.00  0.00           H
ATOM    224 2HE2 GLN N 567      22.514  24.033  10.471  1.00  0.00           H
ATOM    225  N   LEU N 568      19.313  19.365  14.871  1.00 46.05           N
```

FIG. 5D

ATOM	226	CA	LEU	N	568	18.513	18.907	15.980	1.00	47.97	C
ATOM	227	C	LEU	N	568	19.410	18.201	16.958	1.00	47.65	C
ATOM	228	O	LEU	N	568	19.319	18.457	18.167	1.00	48.06	O
ATOM	229	CB	LEU	N	568	17.399	18.019	15.472	1.00	47.11	C
ATOM	230	CG	LEU	N	568	16.441	18.651	14.453	1.00	52.05	C
ATOM	231	CD1	LEU	N	568	15.376	17.669	14.033	1.00	49.38	C
ATOM	232	CD2	LEU	N	568	15.844	19.917	15.044	1.00	53.06	C
ATOM	233	H	LEU	N	568	19.352	18.869	14.024	1.00	0.00	H
ATOM	234	N	THR	N	569	20.343	17.385	16.474	1.00	47.68	N
ATOM	235	CA	THR	N	569	21.300	16.706	17.345	1.00	46.82	C
ATOM	236	C	THR	N	569	22.179	17.733	18.051	1.00	46.78	C
ATOM	237	O	THR	N	569	22.428	17.562	19.238	1.00	46.53	O
ATOM	238	CB	THR	N	569	22.196	15.706	16.513	1.00	48.47	C
ATOM	239	OG1	THR	N	569	22.896	16.453	15.512	1.00	50.39	O
ATOM	240	CG2	THR	N	569	21.367	14.574	15.887	1.00	45.02	C
ATOM	241	H	THR	N	569	20.365	17.208	15.510	1.00	0.00	H
ATOM	242	HG1	THR	N	569	22.309	16.916	14.917	1.00	0.00	H
ATOM	243	N	VAL	N	570	22.568	18.851	17.411	1.00	46.51	N
ATOM	244	CA	VAL	N	570	23.388	19.879	18.056	1.00	46.07	C
ATOM	245	C	VAL	N	570	22.584	20.543	19.173	1.00	46.10	C
ATOM	246	O	VAL	N	570	23.109	20.791	20.268	1.00	46.19	O
ATOM	247	CB	VAL	N	570	23.824	20.975	17.067	1.00	46.87	C
ATOM	248	CG1	VAL	N	570	24.628	22.078	17.767	1.00	43.56	C
ATOM	249	CG2	VAL	N	570	24.698	20.324	16.003	1.00	47.58	C
ATOM	250	H	VAL	N	570	22.267	19.018	16.480	1.00	0.00	H
ATOM	251	N	TRP	N	571	21.311	20.824	18.901	1.00	44.96	N
ATOM	252	CA	TRP	N	571	20.448	21.354	19.916	1.00	45.54	C
ATOM	253	C	TRP	N	571	20.408	20.357	21.079	1.00	45.70	C
ATOM	254	O	TRP	N	571	20.466	20.796	22.237	1.00	46.48	O
ATOM	255	CB	TRP	N	571	19.025	21.547	19.422	1.00	45.68	C
ATOM	256	CG	TRP	N	571	18.046	21.979	20.538	1.00	47.31	C
ATOM	257	CD1	TRP	N	571	17.853	23.309	20.778	1.00	47.86	C
ATOM	258	CD2	TRP	N	571	17.291	21.171	21.401	1.00	48.92	C
ATOM	259	NE1	TRP	N	571	16.991	23.361	21.767	1.00	47.92	N
ATOM	260	CE2	TRP	N	571	16.630	22.132	22.175	1.00	47.99	C
ATOM	261	CE3	TRP	N	571	17.056	19.805	21.674	1.00	48.37	C
ATOM	262	CZ2	TRP	N	571	15.742	21.753	23.189	1.00	46.81	C
ATOM	263	CZ3	TRP	N	571	16.181	19.419	22.697	1.00	46.38	C
ATOM	264	CH2	TRP	N	571	15.524	20.395	23.451	1.00	47.44	C
ATOM	265	H	TRP	N	571	20.993	20.625	17.998	1.00	0.00	H
ATOM	266	HE1	TRP	N	571	16.632	24.201	22.162	1.00	0.00	H
ATOM	267	N	GLY	N	572	20.356	19.036	20.842	1.00	45.29	N
ATOM	268	CA	GLY	N	572	20.270	18.034	21.892	1.00	44.49	C
ATOM	269	C	GLY	N	572	21.532	18.044	22.719	1.00	44.03	C
ATOM	270	O	GLY	N	572	21.491	18.102	23.948	1.00	43.66	O
ATOM	271	H	GLY	N	572	20.483	18.736	19.917	1.00	0.00	H
ATOM	272	N	ILE	N	573	22.671	18.122	22.031	1.00	44.11	N
ATOM	273	CA	ILE	N	573	23.986	18.156	22.666	1.00	44.64	C
ATOM	274	C	ILE	N	573	24.148	19.402	23.527	1.00	45.83	C
ATOM	275	O	ILE	N	573	24.571	19.300	24.666	1.00	46.58	O
ATOM	276	CB	ILE	N	573	25.125	18.159	21.622	1.00	44.82	C
ATOM	277	CG1	ILE	N	573	25.094	16.885	20.810	1.00	43.85	C
ATOM	278	CG2	ILE	N	573	26.482	18.303	22.325	1.00	44.82	C
ATOM	279	CD1	ILE	N	573	26.010	16.983	19.585	1.00	44.87	C
ATOM	280	H	ILE	N	573	22.603	18.229	21.056	1.00	0.00	H
ATOM	281	N	LYS	N	574	23.840	20.594	23.044	1.00	46.57	N
ATOM	282	CA	LYS	N	574	24.001	21.819	23.817	1.00	47.39	C
ATOM	283	C	LYS	N	574	23.075	21.810	25.027	1.00	47.64	C

FIG. 5E

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ATOM    284   O   LYS N 574      23.456  22.221  26.103  1.00 47.42           O
ATOM    285   CB  LYS N 574      23.679  23.041  22.944  1.00 47.81           C
ATOM    286   CG  LYS N 574      24.626  23.233  21.776  1.00 47.81           C
ATOM    287   CD  LYS N 574      24.343  24.597  21.117  1.00 49.66           C
ATOM    288   CE  LYS N 574      25.235  24.786  19.879  1.00 57.06           C
ATOM    289   NZ  LYS N 574      25.047  26.026  19.167  1.00 51.95           N
ATOM    290   H   LYS N 574      23.447  20.634  22.137  1.00  0.00           H
ATOM    291  1HZ  LYS N 574      24.056  26.097  18.850  1.00  0.00           H
ATOM    292  2HZ  LYS N 574      25.302  26.787  19.816  1.00  0.00           H
ATOM    293  3HZ  LYS N 574      25.671  26.035  18.326  1.00  0.00           H
ATOM    294   N   GLN N 575      21.863  21.301  24.898  1.00 47.76           N
ATOM    295   CA  GLN N 575      20.947  21.160  26.010  1.00 49.56           C
ATOM    296   C   GLN N 575      21.523  20.277  27.101  1.00 50.70           C
ATOM    297   O   GLN N 575      21.530  20.599  28.288  1.00 50.85           O
ATOM    298   CB  GLN N 575      19.690  20.480  25.617  1.00 51.27           C
ATOM    299   CG  GLN N 575      18.703  21.312  24.814  1.00 53.77           C
ATOM    300   CD  GLN N 575      18.143  22.472  25.591  1.00 56.45           C
ATOM    301   OE1 GLN N 575      17.537  22.387  26.656  1.00 59.04           O
ATOM    302   NE2 GLN N 575      18.305  23.636  25.024  1.00 57.29           N
ATOM    303   H   GLN N 575      21.606  20.942  24.016  1.00  0.00           H
ATOM    304  1HE2 GLN N 575      17.915  24.394  25.512  1.00  0.00           H
ATOM    305  2HE2 GLN N 575      18.755  23.713  24.154  1.00  0.00           H
ATOM    306   N   LEU N 576      22.054  19.126  26.704  1.00 52.27           N
ATOM    307   CA  LEU N 576      22.609  18.227  27.703  1.00 54.14           C
ATOM    308   C   LEU N 576      23.887  18.797  28.277  1.00 55.59           C
ATOM    309   O   LEU N 576      24.135  18.667  29.472  1.00 55.72           O
ATOM    310   CB  LEU N 576      22.892  16.841  27.117  1.00 51.84           C
ATOM    311   CG  LEU N 576      21.688  16.085  26.553  1.00 52.59           C
ATOM    312   CD1 LEU N 576      22.138  14.746  26.001  1.00 50.01           C
ATOM    313   CD2 LEU N 576      20.643  15.931  27.638  1.00 51.10           C
ATOM    314   H   LEU N 576      22.073  18.904  25.743  1.00  0.00           H
ATOM    315   N   GLN N 577      24.692  19.489  27.474  1.00 57.40           N
ATOM    316   CA  GLN N 577      25.921  20.110  27.929  1.00 59.81           C
ATOM    317   C   GLN N 577      25.672  21.245  28.915  1.00 62.47           C
ATOM    318   O   GLN N 577      26.453  21.404  29.852  1.00 62.30           O
ATOM    319   CB  GLN N 577      26.708  20.620  26.730  1.00 57.05           C
ATOM    320   CG  GLN N 577      28.060  21.087  27.186  1.00 58.22           C
ATOM    321   CD  GLN N 577      28.180  22.600  27.330  1.00 60.01           C
ATOM    322   OE1 GLN N 577      27.202  23.340  27.358  1.00 60.52           O
ATOM    323   NE2 GLN N 577      29.385  23.134  27.363  1.00 61.54           N
ATOM    324   H   GLN N 577      24.455  19.535  26.530  1.00  0.00           H
ATOM    325  1HE2 GLN N 577      29.399  24.107  27.430  1.00  0.00           H
ATOM    326  2HE2 GLN N 577      30.164  22.554  27.335  1.00  0.00           H
ATOM    327   N   ALA N 578      24.584  21.997  28.775  1.00 65.04           N
ATOM    328   CA  ALA N 578      24.312  23.121  29.647  1.00 67.52           C
ATOM    329   C   ALA N 578      24.101  22.643  31.062  1.00 69.93           C
ATOM    330   O   ALA N 578      24.379  23.346  32.025  1.00 70.22           O
ATOM    331   CB  ALA N 578      23.056  23.840  29.207  1.00 66.26           C
ATOM    332   H   ALA N 578      23.987  21.810  28.016  1.00  0.00           H
ATOM    333   N   ARG N 579      23.604  21.407  31.195  1.00 72.80           N
ATOM    334   CA  ARG N 579      23.277  20.834  32.491  1.00 76.15           C
ATOM    335   C   ARG N 579      24.297  19.924  33.116  1.00 77.71           C
ATOM    336   O   ARG N 579      24.155  19.391  34.212  1.00 78.20           O
ATOM    337   CB  ARG N 579      21.939  20.093  32.368  1.00 77.38           C
ATOM    338   CG  ARG N 579      20.802  20.968  31.853  1.00 80.38           C
ATOM    339   CD  ARG N 579      19.487  20.222  31.726  1.00 84.49           C
ATOM    340   NE  ARG N 579      18.438  21.069  31.147  1.00 88.84           N
ATOM    341   CZ  ARG N 579      17.385  20.587  30.457  1.00 91.52           C
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FIG. 5F

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ATOM    342  NH1 ARG N 579      17.230  19.303  30.253  1.00 94.12           N
ATOM    343  NH2 ARG N 579      16.430  21.352  29.931  1.00 90.71           N
ATOM    344  H   ARG N 579      23.402  20.913  30.376  1.00  0.00           H
ATOM    345  HE  ARG N 579      18.509  22.039  31.265  1.00  0.00           H
ATOM    346 1HH1 ARG N 579      17.879  18.631  30.623  1.00  0.00           H
ATOM    347 2HH1 ARG N 579      16.423  18.975  29.754  1.00  0.00           H
ATOM    348 1HH2 ARG N 579      16.473  22.346  30.014  1.00  0.00           H
ATOM    349 2HH2 ARG N 579      15.675  20.923  29.427  1.00  0.00           H
ATOM    350  N   ILE N 580      25.362  19.713  32.371  1.00 79.12           N
ATOM    351  CA  ILE N 580      26.445  18.772  32.675  1.00 81.05           C
ATOM    352  C   ILE N 580      27.660  19.565  32.303  1.00 82.42           C
ATOM    353  O   ILE N 580      28.531  19.018  31.659  1.00 83.59           O
ATOM    354  CB  ILE N 580      26.246  17.503  31.784  1.00 80.80           C
ATOM    355  CG1 ILE N 580      25.193  16.697  32.429  1.00 84.04           C
ATOM    356  CG2 ILE N 580      27.451  16.589  31.650  1.00 78.88           C
ATOM    357  CD1 ILE N 580      24.516  16.191  31.215  1.00 86.00           C
ATOM    358  H   ILE N 580      25.445  20.241  31.548  1.00  0.00           H
ATOM    359  N   LEU N 581      27.698  20.865  32.557  1.00 83.28           N
ATOM    360  CA  LEU N 581      28.887  21.706  32.347  1.00 83.95           C
ATOM    361  C   LEU N 581      28.597  23.173  32.668  1.00 84.95           C
ATOM    362  O   LEU N 581      27.778  23.359  33.577  1.00 88.48           O
ATOM    363  CB  LEU N 581      29.461  21.581  30.920  1.00 82.81           C
ATOM    364  CG  LEU N 581      30.924  21.079  30.935  1.00 80.52           C
ATOM    365  CD1 LEU N 581      31.242  20.050  32.038  1.00 78.52           C
ATOM    366  CD2 LEU N 581      31.148  20.566  29.548  1.00 80.15           C
ATOM    367  H   LEU N 581      26.907  21.292  32.938  1.00  0.00           H
TER     368      LEU N 581
HETATM  369  C   ACE C   0      11.678  19.563  23.916  1.00 59.46           C
HETATM  370  O   ACE C   0      11.509  19.280  22.723  1.00 59.59           O
HETATM  371  CH3 ACE C   0      11.401  20.961  24.478  1.00 59.14           C
ATOM    372  N   TRP C 628      11.939  18.567  24.754  1.00 59.45           N
ATOM    373  CA  TRP C 628      12.345  17.262  24.249  1.00 58.85           C
ATOM    374  C   TRP C 628      11.305  16.438  23.468  1.00 59.28           C
ATOM    375  O   TRP C 628      11.646  15.639  22.589  1.00 59.31           O
ATOM    376  CB  TRP C 628      12.905  16.491  25.449  1.00 56.27           C
ATOM    377  CG  TRP C 628      14.324  16.987  25.710  1.00 52.28           C
ATOM    378  CD1 TRP C 628      14.560  17.945  26.654  1.00 52.77           C
ATOM    379  CD2 TRP C 628      15.466  16.576  25.059  1.00 52.52           C
ATOM    380  NE1 TRP C 628      15.852  18.149  26.605  1.00 53.20           N
ATOM    381  CE2 TRP C 628      16.442  17.360  25.680  1.00 53.25           C
ATOM    382  CE3 TRP C 628      15.833  15.676  24.060  1.00 49.19           C
ATOM    383  CZ2 TRP C 628      17.793  17.256  25.297  1.00 50.70           C
ATOM    384  CZ3 TRP C 628      17.180  15.570  23.699  1.00 49.98           C
ATOM    385  CH2 TRP C 628      18.158  16.350  24.304  1.00 47.48           C
ATOM    386  H   TRP C 628      11.881  18.708  25.724  1.00  0.00           H
ATOM    387  HE1 TRP C 628      16.338  18.759  27.208  1.00  0.00           H
ATOM    388  N   MET C 629       9.992  16.635  23.651  1.00 59.74           N
ATOM    389  CA  MET C 629       9.041  15.870  22.852  1.00 60.58           C
ATOM    390  C   MET C 629       8.978  16.434  21.441  1.00 59.92           C
ATOM    391  O   MET C 629       8.878  15.698  20.450  1.00 59.94           O
ATOM    392  CB  MET C 629       7.644  15.848  23.489  1.00 63.71           C
ATOM    393  CG  MET C 629       7.364  16.823  24.657  1.00 68.98           C
ATOM    394  SD  MET C 629       6.220  16.291  25.948  1.00 72.59           S
ATOM    395  CE  MET C 629       4.843  16.119  24.844  1.00 72.83           C
ATOM    396  H   MET C 629       9.728  17.227  24.356  1.00  0.00           H
ATOM    397  N   GLU C 630       9.151  17.749  21.302  1.00 59.19           N
ATOM    398  CA  GLU C 630       9.179  18.350  19.990  1.00 59.94           C
ATOM    399  C   GLU C 630      10.391  17.903  19.195  1.00 59.73           C
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FIG. 5G

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ATOM    400  O   GLU C 630      10.317  17.666  17.988  1.00 58.71           O
ATOM    401  CB  GLU C 630       9.192  19.876  20.063  1.00 62.30           C
ATOM    402  CG  GLU C 630       9.263  20.558  18.693  1.00 66.55           C
ATOM    403  CD  GLU C 630       8.214  20.271  17.616  1.00 69.57           C
ATOM    404  OE1 GLU C 630       7.325  19.430  17.788  1.00 71.12           O
ATOM    405  OE2 GLU C 630       8.304  20.921  16.577  1.00 71.20           O
ATOM    406  H   GLU C 630       9.289  18.287  22.086  1.00  0.00           H
ATOM    407  N   TRP C 631      11.517  17.795  19.893  1.00 60.09           N
ATOM    408  CA  TRP C 631      12.758  17.353  19.309  1.00 60.33           C
ATOM    409  C   TRP C 631      12.541  15.931  18.819  1.00 61.17           C
ATOM    410  O   TRP C 631      12.869  15.598  17.708  1.00 61.33           O
ATOM    411  CB  TRP C 631      13.836  17.478  20.395  1.00 56.29           C
ATOM    412  CG  TRP C 631      15.206  16.925  19.960  1.00 54.47           C
ATOM    413  CD1 TRP C 631      16.103  17.708  19.291  1.00 54.11           C
ATOM    414  CD2 TRP C 631      15.644  15.637  20.169  1.00 50.58           C
ATOM    415  NE1 TRP C 631      17.137  16.928  19.120  1.00 53.39           N
ATOM    416  CE2 TRP C 631      16.924  15.687  19.621  1.00 50.81           C
ATOM    417  CE3 TRP C 631      15.169  14.490  20.782  1.00 44.66           C
ATOM    418  CZ2 TRP C 631      17.755  14.558  19.662  1.00 48.32           C
ATOM    419  CZ3 TRP C 631      15.995  13.360  20.809  1.00 45.04           C
ATOM    420  CH2 TRP C 631      17.274  13.377  20.242  1.00 45.24           C
ATOM    421  H   TRP C 631      11.515  18.006  20.858  1.00  0.00           H
ATOM    422  HE1 TRP C 631      17.965  17.239  18.688  1.00  0.00           H
ATOM    423  N   ASP C 632      11.873  15.089  19.562  1.00 62.54           N
ATOM    424  CA  ASP C 632      11.600  13.733  19.160  1.00 64.59           C
ATOM    425  C   ASP C 632      10.784  13.653  17.877  1.00 65.43           C
ATOM    426  O   ASP C 632      11.049  12.839  16.989  1.00 65.87           O
ATOM    427  CB  ASP C 632      10.801  13.059  20.184  1.00 66.75           C
ATOM    428  CG  ASP C 632      11.553  11.867  20.759  1.00 70.81           C
ATOM    429  OD1 ASP C 632      11.763  10.875  20.036  1.00 73.19           O
ATOM    430  OD2 ASP C 632      11.864  12.009  21.934  1.00 73.17           O
ATOM    431  H   ASP C 632      11.482  15.413  20.422  1.00  0.00           H
ATOM    432  N   ARG C 633       9.741  14.481  17.788  1.00 65.95           N
ATOM    433  CA  ARG C 633       8.846  14.452  16.645  1.00 66.10           C
ATOM    434  C   ARG C 633       9.628  15.030  15.464  1.00 64.57           C
ATOM    435  O   ARG C 633       9.583  14.449  14.377  1.00 64.74           O
ATOM    436  CB  ARG C 633       7.586  15.329  16.804  1.00 70.93           C
ATOM    437  CG  ARG C 633       6.473  15.063  17.832  1.00 77.51           C
ATOM    438  CD  ARG C 633       5.742  16.383  18.096  1.00 83.59           C
ATOM    439  NE  ARG C 633       5.101  16.320  19.404  1.00 90.92           N
ATOM    440  CZ  ARG C 633       3.946  16.916  19.715  1.00 96.53           C
ATOM    441  NH1 ARG C 633       3.295  17.634  18.820  1.00 99.82           N
ATOM    442  NH2 ARG C 633       3.344  16.753  20.891  1.00 99.12           N
ATOM    443  H   ARG C 633       9.604  15.123  18.523  1.00  0.00           H
ATOM    444  HE  ARG C 633       5.536  15.785  20.096  1.00  0.00           H
ATOM    445 1HH1 ARG C 633       3.715  17.801  17.918  1.00  0.00           H
ATOM    446 2HH1 ARG C 633       2.486  18.174  19.079  1.00  0.00           H
ATOM    447 1HH2 ARG C 633       3.713  16.130  21.573  1.00  0.00           H
ATOM    448 2HH2 ARG C 633       2.491  17.256  21.077  1.00  0.00           H
ATOM    449  N   GLU C 634      10.397  16.100  15.645  1.00 62.76           N
ATOM    450  CA  GLU C 634      11.159  16.676  14.569  1.00 61.33           C
ATOM    451  C   GLU C 634      12.229  15.727  14.081  1.00 60.46           C
ATOM    452  O   GLU C 634      12.486  15.655  12.877  1.00 61.42           O
ATOM    453  CB  GLU C 634      11.823  17.935  14.998  1.00 61.32           C
ATOM    454  CG  GLU C 634      10.784  19.053  14.903  1.00 68.08           C
ATOM    455  CD  GLU C 634      11.401  20.433  14.751  1.00 74.96           C
ATOM    456  OE1 GLU C 634      12.353  20.598  13.977  1.00 76.47           O
ATOM    457  OE2 GLU C 634      10.902  21.363  15.384  1.00 77.59           O
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FIG. 5H

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ATOM    458  H   GLU C 634      10.437  16.483  16.554  1.00  0.00      H
ATOM    459  N   ILE C 635      12.783  14.913  14.993  1.00 59.27      N
ATOM    460  CA  ILE C 635      13.782  13.906  14.663  1.00 56.77      C
ATOM    461  C   ILE C 635      13.110  12.816  13.854  1.00 57.26      C
ATOM    462  O   ILE C 635      13.714  12.292  12.927  1.00 56.53      O
ATOM    463  CB  ILE C 635      14.429  13.299  15.953  1.00 52.95      C
ATOM    464  CG1 ILE C 635      15.236  14.321  16.698  1.00 47.91      C
ATOM    465  CG2 ILE C 635      15.388  12.182  15.569  1.00 52.10      C
ATOM    466  CD1 ILE C 635      16.358  14.961  15.927  1.00 50.08      C
ATOM    467  H   ILE C 635      12.540  15.067  15.936  1.00  0.00      H
ATOM    468  N   ASN C 636      11.854  12.452  14.086  1.00 58.11      N
ATOM    469  CA  ASN C 636      11.273  11.345  13.347  1.00 58.91      C
ATOM    470  C   ASN C 636      10.775  11.849  12.030  1.00 59.34      C
ATOM    471  O   ASN C 636      10.926  11.176  11.020  1.00 59.71      O
ATOM    472  CB  ASN C 636      10.132  10.719  14.134  1.00 59.74      C
ATOM    473  CG  ASN C 636      10.632  10.044  15.400  1.00 61.95      C
ATOM    474  OD1 ASN C 636      11.698   9.427  15.428  1.00 65.00      O
ATOM    475  ND2 ASN C 636       9.938  10.198  16.516  1.00 60.78      N
ATOM    476  H   ASN C 636      11.345  12.892  14.807  1.00  0.00      H
ATOM    477 1HD2 ASN C 636      10.323   9.834  17.341  1.00  0.00      H
ATOM    478 2HD2 ASN C 636       9.118  10.706  16.495  1.00  0.00      H
ATOM    479  N   ASN C 637      10.278  13.076  12.015  1.00 59.84      N
ATOM    480  CA  ASN C 637       9.779  13.751  10.816  1.00 61.12      C
ATOM    481  C   ASN C 637      10.834  13.839   9.723  1.00 61.25      C
ATOM    482  O   ASN C 637      10.585  13.594   8.538  1.00 61.53      O
ATOM    483  CB  ASN C 637       9.383  15.219  11.029  1.00 64.01      C
ATOM    484  CG  ASN C 637       8.112  15.513  11.887  1.00 67.80      C
ATOM    485  OD1 ASN C 637       7.302  14.605  12.111  1.00 68.43      O
ATOM    486  ND2 ASN C 637       7.948  16.748  12.355  1.00 68.62      N
ATOM    487  H   ASN C 637      10.230  13.550  12.877  1.00  0.00      H
ATOM    488 1HD2 ASN C 637       7.144  16.914  12.846  1.00  0.00      H
ATOM    489 2HD2 ASN C 637       8.650  17.412  12.187  1.00  0.00      H
ATOM    490  N   TYR C 638      12.033  14.300  10.102  1.00 60.30      N
ATOM    491  CA  TYR C 638      13.127  14.392   9.169  1.00 58.95      C
ATOM    492  C   TYR C 638      13.679  13.029   8.854  1.00 58.12      C
ATOM    493  O   TYR C 638      14.008  12.788   7.698  1.00 58.25      O
ATOM    494  CB  TYR C 638      14.165  15.327   9.774  1.00 58.34      C
ATOM    495  CG  TYR C 638      13.667  16.749   9.673  1.00 58.76      C
ATOM    496  CD1 TYR C 638      13.303  17.225   8.418  1.00 59.13      C
ATOM    497  CD2 TYR C 638      13.521  17.567  10.800  1.00 59.56      C
ATOM    498  CE1 TYR C 638      12.850  18.517   8.256  1.00 58.59      C
ATOM    499  CE2 TYR C 638      13.091  18.900  10.637  1.00 60.72      C
ATOM    500  CZ  TYR C 638      12.738  19.343   9.354  1.00 59.43      C
ATOM    501  OH  TYR C 638      12.451  20.666   9.088  1.00 58.81      O
ATOM    502  H   TYR C 638      12.162  14.682  11.009  1.00  0.00      H
ATOM    503  HH  TYR C 638      12.351  20.876   8.165  1.00  0.00      H
ATOM    504  N   THR C 639      13.706  12.108   9.796  1.00 57.10      N
ATOM    505  CA  THR C 639      14.134  10.771   9.461  1.00 57.84      C
ATOM    506  C   THR C 639      13.232  10.085   8.424  1.00 58.82      C
ATOM    507  O   THR C 639      13.725   9.331   7.554  1.00 58.69      O
ATOM    508  CB  THR C 639      14.163   9.904  10.683  1.00 57.69      C
ATOM    509  OG1 THR C 639      15.110  10.474  11.544  1.00 60.10      O
ATOM    510  CG2 THR C 639      14.597   8.478  10.387  1.00 55.45      C
ATOM    511  H   THR C 639      13.402  12.348  10.690  1.00  0.00      H
ATOM    512  HG1 THR C 639      14.818  11.323  11.889  1.00  0.00      H
ATOM    513  N   SER C 640      11.916  10.315   8.505  1.00 59.42      N
ATOM    514  CA  SER C 640      10.997   9.745   7.531  1.00 60.07      C
ATOM    515  C   SER C 640      11.177  10.391   6.160  1.00 58.97      C
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FIG. 5I

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ATOM    516  O   SER C 640      11.169   9.642   5.177  1.00 60.33           O
ATOM    517  CB  SER C 640       9.549   9.934   7.966  1.00 62.43           C
ATOM    518  OG  SER C 640       9.343   9.238   9.188  1.00 69.53           O
ATOM    519  H   SER C 640      11.544  10.854   9.240  1.00  0.00           H
ATOM    520  HG  SER C 640       9.444   8.298   9.074  1.00  0.00           H
ATOM    521  N   LEU C 641      11.375  11.710   6.057  1.00 56.88           N
ATOM    522  CA  LEU C 641      11.619  13.351   4.785  1.00 55.95           C
ATOM    523  C   LEU C 641      12.948  11.832   4.190  1.00 56.33           C
ATOM    524  O   LEU C 641      13.039  11.552   2.988  1.00 55.67           O
ATOM    525  CB  LEU C 641      11.658  13.879   5.006  1.00 53.81           C
ATOM    526  CG  LEU C 641      11.718  14.767   3.765  1.00 52.82           C
ATOM    527  CD1 LEU C 641      10.375  14.703   3.035  1.00 52.33           C
ATOM    528  CD2 LEU C 641      12.047  16.198   4.163  1.00 50.59           C
ATOM    529  H   LEU C 641      11.357  12.252   6.875  1.00  0.00           H
ATOM    530  N   ILE C 642      13.988  11.612   5.019  1.00 55.99           N
ATOM    531  CA  ILE C 642      15.290  11.153   4.549  1.00 55.40           C
ATOM    532  C   ILE C 642      15.163   9.729   4.112  1.00 55.08           C
ATOM    533  O   ILE C 642      15.740   9.343   3.115  1.00 55.36           O
ATOM    534  CB  ILE C 642      16.384  11.240   5.647  1.00 54.86           C
ATOM    535  CG1 ILE C 642      16.630  12.661   6.041  1.00 53.06           C
ATOM    536  CG2 ILE C 642      17.722  10.778   5.097  1.00 57.37           C
ATOM    537  CD1 ILE C 642      17.486  12.825   7.287  1.00 48.58           C
ATOM    538  H   ILE C 642      13.884  11.813   5.980  1.00  0.00           H
ATOM    539  N   HIS C 643      14.415   8.904   4.785  1.00 55.14           N
ATOM    540  CA  HIS C 643      14.197   7.568   4.260  1.00 56.94           C
ATOM    541  C   HIS C 643      13.527   7.512   2.940  1.00 55.82           C
ATOM    542  O   HIS C 643      13.928   6.699   2.100  1.00 55.49           O
ATOM    543  CB  HIS C 643      13.347   6.771   5.191  1.00 63.78           C
ATOM    544  CG  HIS C 643      14.340   6.051   6.088  1.00 73.07           C
ATOM    545  ND1 HIS C 643      14.544   4.739   6.144  1.00 78.26           N
ATOM    546  CD2 HIS C 643      15.193   6.704   6.938  1.00 77.77           C
ATOM    547  CE1 HIS C 643      15.501   4.583   6.998  1.00 81.50           C
ATOM    548  NE2 HIS C 643      15.885   5.758   7.472  1.00 81.84           N
ATOM    549  H   HIS C 643      13.952   9.236   8.598  1.00  0.00           H
ATOM    550  HD1 HIS C 643      14.017   4.059   5.688  1.00  0.00           H
ATOM    551  HE2 HIS C 643      16.617   5.921   8.100  1.00  0.00           H
ATOM    552  N   SER C 644      12.503   8.344   2.761  1.00 55.58           N
ATOM    553  CA  SER C 644      11.826   8.384   1.478  1.00 54.97           C
ATOM    554  C   SER C 644      13.782   8.888   0.398  1.00 53.50           C
ATOM    555  O   SER C 644      12.797   8.293  -0.691  1.00 53.52           O
ATOM    556  CB  SER C 644      10.644   9.369   1.377  1.00 56.29           C
ATOM    557  OG  SER C 644       9.823   9.759   2.572  1.00 59.92           O
ATOM    558  H   SER C 644      13.128   8.851   3.524  1.00  0.00           H
ATOM    559  HG  SER C 644       9.441   8.970   2.959  1.00  0.00           H
ATOM    560  N   LEU C 645      13.612   9.918   0.673  1.00 51.33           N
ATOM    561  CA  LEU C 645      14.485  10.438  -0.351  1.00 48.71           C
ATOM    562  C   LEU C 645      15.593   9.476  -0.651  1.00 49.35           C
ATOM    563  O   LEU C 645      15.914   9.316  -1.820  1.00 49.33           O
ATOM    564  CB  LEU C 645      15.027  11.807   0.080  1.00 45.58           C
ATOM    565  CG  LEU C 645      13.979  12.903   0.305  1.00 39.61           C
ATOM    566  CD1 LEU C 645      14.665  14.149   0.710  1.00 41.30           C
ATOM    567  CD2 LEU C 645      13.200  13.183  -0.954  1.00 38.15           C
ATOM    568  H   LEU C 645      13.620  10.325   1.566  1.00  0.00           H
ATOM    569  N   ILE C 646      16.114   8.734   0.334  1.00 48.24           N
ATOM    570  CA  ILE C 646      17.178   7.748   0.106  1.00 48.80           C
ATOM    571  C   ILE C 646      16.595   6.620  -0.736  1.00 51.17           C
ATOM    572  O   ILE C 646      17.236   6.140  -1.676  1.00 50.43           O
ATOM    573  CB  ILE C 646      17.720   7.222   1.450  1.00 44.77           C
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FIG. 5J

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ATOM    574  CG1 ILE C 646      18.414   8.325   2.218  1.00 43.19           C
ATOM    575  CG2 ILE C 646      18.745   6.158   1.182  1.00 43.97           C
ATOM    576  CD1 ILE C 646      18.854   7.897   3.621  1.00 39.46           C
ATOM    577  H   ILE C 646      15.785   8.879   1.246  1.00  0.00           H
ATOM    578  N   GLU C 647      15.348   6.236  -0.482  1.00 54.35           N
ATOM    579  CA  GLU C 647      14.685   5.186  -1.244  1.00 56.99           C
ATOM    580  C   GLU C 647      14.377   5.647  -2.682  1.00 57.37           C
ATOM    581  O   GLU C 647      14.604   4.923  -3.662  1.00 58.06           O
ATOM    582  CB  GLU C 647      13.408   4.828  -0.527  1.00 62.05           C
ATOM    583  CG  GLU C 647      12.691   3.564  -1.047  1.00 71.88           C
ATOM    584  CD  GLU C 647      11.372   3.218  -0.346  1.00 79.96           C
ATOM    585  OE1 GLU C 647      10.947   3.931   0.578  1.00 83.26           O
ATOM    586  OE2 GLU C 647      10.766   2.217  -0.738  1.00 83.60           O
ATOM    587  H   GLU C 647      14.843   6.711   0.208  1.00  0.00           H
ATOM    588  N   GLU C 648      13.876   6.871  -2.874  1.00 57.16           N
ATOM    589  CA  GLU C 648      13.588   7.431  -4.178  1.00 57.13           C
ATOM    590  C   GLU C 648      14.863   7.517  -4.984  1.00 55.73           C
ATOM    591  O   GLU C 648      14.864   7.188  -6.175  1.00 55.55           O
ATOM    592  CB  GLU C 648      13.051   8.796  -4.039  1.00 62.05           C
ATOM    593  CG  GLU C 648      12.503   9.437  -5.318  1.00 74.11           C
ATOM    594  CD  GLU C 648      11.969  10.872  -5.126  1.00 85.94           C
ATOM    595  OE1 GLU C 648      11.991  11.409  -4.008  1.00 91.79           O
ATOM    596  OE2 GLU C 648      11.521  11.471  -6.110  1.00 88.20           O
ATOM    597  H   GLU C 648      13.711   7.409  -2.074  1.00  0.00           H
ATOM    598  N   SER C 649      15.950   7.961  -4.364  1.00 54.84           N
ATOM    599  CA  SER C 649      17.251   8.032  -4.994  1.00 53.47           C
ATOM    600  C   SER C 649      17.811   6.694  -5.403  1.00 52.80           C
ATOM    601  O   SER C 649      18.368   6.564  -6.482  1.00 53.07           O
ATOM    602  CB  SER C 649      18.191   8.704  -4.055  1.00 52.08           C
ATOM    603  OG  SER C 649      17.841  10.043  -3.742  1.00 48.93           O
ATOM    604  H   SER C 649      15.881   8.274  -3.436  1.00  0.00           H
ATOM    605  HG  SER C 649      17.888  10.547  -4.561  1.00  0.00           H
ATOM    606  N   GLN C 650      17.622   5.684  -4.563  1.00 52.79           N
ATOM    607  CA  GLN C 650      17.985   4.285  -4.808  1.00 53.64           C
ATOM    608  C   GLN C 650      17.303   3.776  -6.071  1.00 53.04           C
ATOM    609  O   GLN C 650      17.951   3.085  -6.882  1.00 54.05           O
ATOM    610  CB  GLN C 650      17.547   3.387  -3.634  1.00 56.65           C
ATOM    611  CG  GLN C 650      18.565   2.745  -2.685  1.00 62.17           C
ATOM    612  CD  GLN C 650      17.982   2.264  -1.334  1.00 66.78           C
ATOM    613  OE1 GLN C 650      16.991   1.535  -1.224  1.00 69.78           O
ATOM    614  NE2 GLN C 650      18.538   2.637  -0.192  1.00 67.82           N
ATOM    615  H   GLN C 650      17.260   5.899  -3.670  1.00  0.00           H
ATOM    616 1HE2 GLN C 650      18.083   2.295   0.609  1.00  0.00           H
ATOM    617 2HE2 GLN C 650      19.324   3.204  -0.193  1.00  0.00           H
ATOM    618  N   ASN C 651      16.035   4.183  -6.268  1.00 51.27           N
ATOM    619  CA  ASN C 651      15.261   3.761  -7.435  1.00 49.91           C
ATOM    620  C   ASN C 651      15.708   4.500  -8.681  1.00 48.34           C
ATOM    621  O   ASN C 651      15.988   3.912  -9.726  1.00 47.51           O
ATOM    622  CB  ASN C 651      13.776   4.018  -7.246  1.00 49.79           C
ATOM    623  CG  ASN C 651      13.276   3.154  -6.125  1.00 53.41           C
ATOM    624  OD1 ASN C 651      13.709   2.010  -5.961  1.00 52.64           O
ATOM    625  ND2 ASN C 651      12.418   3.728  -5.276  1.00 59.61           N
ATOM    626  H   ASN C 651      15.627   4.783  -5.608  1.00  0.00           H
ATOM    627 1HD2 ASN C 651      12.154   3.212  -4.475  1.00  0.00           H
ATOM    628 2HD2 ASN C 651      12.157   4.647  -5.399  1.00  0.00           H
ATOM    629  N   GLN C 652      15.864   5.821  -8.587  1.00 47.33           N
ATOM    630  CA  GLN C 652      16.350   6.623  -9.690  1.00 47.23           C
ATOM    631  C   GLN C 652      17.758   6.187 -10.002  1.00 47.47           C
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FIG. 5K

ATOM	632	O	GLN	C	652	18.093	6.195	-11.164	1.00	48.04	O
ATOM	633	CB	GLN	C	652	16.307	8.040	-9.279	1.00	45.56	C
ATOM	634	CG	GLN	C	652	16.453	9.174	-10.302	1.00	47.99	C
ATOM	635	CD	GLN	C	652	15.382	9.271	-11.366	1.00	51.30	C
ATOM	636	OE1	GLN	C	652	14.275	9.750	-11.134	1.00	51.42	O
ATOM	637	NE2	GLN	C	652	15.688	8.915	-12.603	1.00	47.15	N
ATOM	638	H	GLN	C	652	15.598	6.247	-7.749	1.00	0.00	H
ATOM	639	1HE2	GLN	C	652	14.985	8.988	-13.303	1.00	0.00	H
ATOM	640	2HE2	GLN	C	652	16.588	8.582	-12.832	1.00	0.00	H
ATOM	641	N	GLN	C	653	18.596	5.741	-9.080	1.00	47.45	N
ATOM	642	CA	GLN	C	653	19.926	5.262	-9.403	1.00	49.03	C
ATOM	643	C	GLN	C	653	19.851	4.058	-10.322	1.00	51.89	C
ATOM	644	O	GLN	C	653	20.554	4.029	-11.335	1.00	52.35	O
ATOM	645	CB	GLN	C	653	20.669	4.856	-8.157	1.00	47.54	C
ATOM	646	CG	GLN	C	653	22.164	4.660	-8.449	1.00	46.28	C
ATOM	647	CD	GLN	C	653	22.929	5.903	-8.922	1.00	45.38	C
ATOM	648	OE1	GLN	C	653	22.474	7.036	-8.956	1.00	45.74	O
ATOM	649	NE2	GLN	C	653	24.191	5.913	-9.220	1.00	45.80	N
ATOM	650	H	GLN	C	653	18.285	5.717	-8.155	1.00	0.00	H
ATOM	651	1HE2	GLN	C	653	24.602	6.803	-9.348	1.00	0.00	H
ATOM	652	2HE2	GLN	C	653	24.738	5.108	-9.124	1.00	0.00	H
ATOM	653	N	GLU	C	654	18.952	3.102	-10.025	1.00	54.43	N
ATOM	654	CA	GLU	C	654	18.763	1.932	-10.883	1.00	55.77	C
ATOM	655	C	GLU	C	654	18.222	2.339	-12.253	1.00	55.11	C
ATOM	656	O	GLU	C	654	18.762	1.916	-13.285	1.00	55.24	O
ATOM	657	CB	GLU	C	654	17.815	0.928	-10.199	1.00	59.12	C
ATOM	658	CG	GLU	C	654	18.515	0.035	-9.155	1.00	69.14	C
ATOM	659	CD	GLU	C	654	17.642	-0.522	-8.002	1.00	76.48	C
ATOM	660	OE1	GLU	C	654	17.220	0.245	-7.134	1.00	77.99	O
ATOM	661	OE2	GLU	C	654	17.376	-1.728	-7.946	1.00	78.90	O
ATOM	662	H	GLU	C	654	18.388	3.228	-9.231	1.00	0.00	H
ATOM	663	N	LYS	C	655	17.219	3.226	-12.313	1.00	54.37	N
ATOM	664	CA	LYS	C	655	16.635	3.697	-13.564	1.00	54.47	C
ATOM	665	C	LYS	C	655	17.643	4.441	-14.445	1.00	54.88	C
ATOM	666	O	LYS	C	655	17.713	4.286	-15.665	1.00	54.37	O
ATOM	667	CB	LYS	C	655	15.456	4.583	-13.204	1.00	54.89	C
ATOM	668	CG	LYS	C	655	14.495	4.868	-14.361	1.00	59.61	C
ATOM	669	CD	LYS	C	655	13.201	5.577	-13.910	1.00	65.23	C
ATOM	670	CE	LYS	C	655	12.251	4.748	-13.002	1.00	68.13	C
ATOM	671	NZ	LYS	C	655	10.937	5.360	-12.806	1.00	69.83	N
ATOM	672	H	LYS	C	655	16.858	3.551	-11.458	1.00	0.00	H
ATOM	673	1HZ	LYS	C	655	11.029	6.298	-12.366	1.00	0.00	H
ATOM	674	2HZ	LYS	C	655	10.454	5.475	-13.724	1.00	0.00	H
ATOM	675	3HZ	LYS	C	655	10.344	4.756	-12.200	1.00	0.00	H
ATOM	676	N	ASN	C	656	18.474	5.275	-13.838	1.00	56.18	N
ATOM	677	CA	ASN	C	656	19.463	6.063	-14.534	1.00	56.44	C
ATOM	678	C	ASN	C	656	20.510	5.128	-15.026	1.00	57.72	C
ATOM	679	O	ASN	C	656	20.860	5.283	-16.194	1.00	58.23	O
ATOM	680	CB	ASN	C	656	20.117	7.094	-13.615	1.00	56.38	C
ATOM	681	CG	ASN	C	656	19.142	8.214	-13.246	1.00	57.60	C
ATOM	682	OD1	ASN	C	656	18.270	8.618	-14.035	1.00	59.08	O
ATOM	683	ND2	ASN	C	656	19.141	8.698	-12.009	1.00	57.31	N
ATOM	684	H	ASN	C	656	18.353	5.436	-12.874	1.00	0.00	H
ATOM	685	1HD2	ASN	C	656	18.438	9.305	-11.726	1.00	0.00	H
ATOM	686	2HD2	ASN	C	656	19.787	8.297	-11.386	1.00	0.00	H
ATOM	687	N	GLU	C	657	20.960	4.129	-14.248	1.00	58.95	N
ATOM	688	CA	GLU	C	657	21.918	3.154	-14.752	1.00	61.26	C
ATOM	689	C	GLU	C	657	21.326	2.381	-15.914	1.00	62.47	C

FIG. 5L

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ATOM    690  O   GLU C 657      21.999   2.178 -16.920  1.00 62.52           O
ATOM    691  CB  GLU C 657      22.297   2.184 -13.687  1.00 62.42           C
ATOM    692  CG  GLU C 657      23.051   2.811 -12.514  1.00 65.99           C
ATOM    693  CD  GLU C 657      23.410   1.852 -11.389  1.00 68.51           C
ATOM    694  OE1 GLU C 657      23.152   0.650 -11.481  1.00 72.44           O
ATOM    695  OE2 GLU C 657      23.970   2.322 -10.407  1.00 69.49           O
ATOM    696  H   GLU C 657      20.656   4.056 -13.317  1.00  0.00           H
ATOM    697  N   GLN C 658      20.051   1.999 -15.851  1.00 63.77           N
ATOM    698  CA  GLN C 658      19.379   1.342 -16.972  1.00 64.97           C
ATOM    699  C   GLN C 658      19.373   2.235 -18.211  1.00 64.88           C
ATOM    700  O   GLN C 658      19.620   1.701 -19.282  1.00 64.89           O
ATOM    701  CB  GLN C 658      17.908   1.040 -16.710  1.00 67.79           C
ATOM    702  CG  GLN C 658      17.473   0.109 -15.580  1.00 69.56           C
ATOM    703  CD  GLN C 658      15.981   0.184 -15.253  1.00 71.90           C
ATOM    704  OE1 GLN C 658      15.214   1.130 -15.491  1.00 69.19           O
ATOM    705  NE2 GLN C 658      15.580  -0.892 -14.597  1.00 73.46           N
ATOM    706  H   GLN C 658      19.527   2.154 -15.036  1.00  0.00           H
ATOM    707 1HE2 GLN C 658      14.637  -0.917 -14.331  1.00  0.00           H
ATOM    708 2HE2 GLN C 658      16.241  -1.579 -14.383  1.00  0.00           H
ATOM    709  N   GLU C 659      19.099   3.533 -18.086  1.00 64.42           N
ATOM    710  CA  GLU C 659      19.001   4.408 -19.239  1.00 64.32           C
ATOM    711  C   GLU C 659      20.328   4.664 -19.917  1.00 62.40           C
ATOM    712  O   GLU C 659      20.389   5.040 -21.080  1.00 61.69           O
ATOM    713  CB  GLU C 659      18.413   5.726 -18.809  1.00 68.95           C
ATOM    714  CG  GLU C 659      18.001   6.640 -19.976  1.00 78.11           C
ATOM    715  CD  GLU C 659      17.379   7.956 -19.530  1.00 86.51           C
ATOM    716  OE1 GLU C 659      17.214   8.159 -18.321  1.00 90.49           O
ATOM    717  OE2 GLU C 659      17.049   8.781 -20.388  1.00 90.41           O
ATOM    718  H   GLU C 659      18.930   3.898 -17.190  1.00  0.00           H
ATOM    719  N   LEU C 660      21.374   4.592 -19.120  1.00 61.04           N
ATOM    720  CA  LEU C 660      22.691   4.691 -19.683  1.00 60.69           C
ATOM    721  C   LEU C 660      23.036   3.531 -20.613  1.00 60.42           C
ATOM    722  O   LEU C 660      23.705   3.774 -21.615  1.00 60.27           O
ATOM    723  CB  LEU C 660      22.697   4.805 -18.521  1.00 60.36           C
ATOM    724  CG  LEU C 660      24.642   6.019 -18.618  1.00 59.86           C
ATOM    725  CD1 LEU C 660      23.883   7.314 -18.999  1.00 64.42           C
ATOM    726  CD2 LEU C 660      25.334   6.131 -17.317  1.00 55.37           C
ATOM    727  H   LEU C 660      21.231   4.584 -18.144  1.00  0.00           H
ATOM    728  N   LEU C 661      22.575   2.323 -20.325  1.00 60.33           N
ATOM    729  CA  LEU C 661      22.856   1.140 -21.141  1.00 60.95           C
ATOM    730  C   LEU C 661      22.049   0.974 -22.446  1.00 61.99           C
ATOM    731  O   LEU C 661      20.871   1.318 -22.502  1.00 60.13           O
ATOM    732  CB  LEU C 661      22.646  -0.115 -20.264  1.00 59.85           C
ATOM    733  CG  LEU C 661      23.452  -0.260 -18.988  1.00 57.97           C
ATOM    734  CD1 LEU C 661      23.106  -1.535 -18.261  1.00 57.79           C
ATOM    735  CD2 LEU C 661      24.896  -0.304 -19.360  1.00 54.71           C
ATOM    736  H   LEU C 661      21.881   2.223 -19.630  1.00  0.00           H
TER     737      LEU C 661
HETATM  738  O   HOH     1      20.374  11.213 -18.121  1.00 71.66           O
HETATM  739 1H   HOH     1      20.431  10.325 -18.535  1.00  0.00           H
HETATM  740 2H   HOH     1      19.472  11.248 -17.822  1.00  0.00           H
HETATM  741  O   HOH     2      21.271   8.706 -17.797  1.00 41.79           O
HETATM  742 1H   HOH     2      21.310   7.838 -17.376  1.00  0.00           H
HETATM  743 2H   HOH     2      22.207   8.971 -17.787  1.00  0.00           H
HETATM  744  O   HOH     3      20.650   1.729  -6.022  1.00 46.90           O
HETATM  745 1H   HOH     3      19.744   1.986  -6.245  1.00  0.00           H
HETATM  746 2H   HOH     3      21.074   2.571  -5.777  1.00  0.00           H
HETATM  747  O   HOH     4      22.303   1.121  -8.408  1.00 60.62           O
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FIG. 5M

HETATM	748	1H	HOH	4	22.825	1.923	-8.306	1.00	0.00	H
HETATM	749	2H	HOH	4	21.811	1.091	-7.565	1.00	0.00	H
HETATM	750	O	HOH	5	12.657	5.253	8.200	1.00	56.12	O
HETATM	751	1H	HOH	5	12.382	4.344	8.353	1.00	0.00	H
HETATM	752	2H	HOH	5	11.869	5.752	8.457	1.00	0.00	H
HETATM	753	O	HOH	6	9.078	18.813	26.094	1.00	49.33	O
HETATM	754	1H	HOH	6	9.131	17.970	25.664	1.00	0.00	H
HETATM	755	2H	HOH	6	9.244	19.463	25.419	1.00	0.00	H
HETATM	756	O	HOH	7	7.670	21.185	11.788	1.00	53.95	O
HETATM	757	1H	HOH	7	7.025	21.036	12.470	1.00	0.00	H
HETATM	758	2H	HOH	7	8.510	21.265	12.230	1.00	0.00	H
HETATM	759	O	HOH	8	8.303	19.620	23.607	1.00	92.51	O
HETATM	760	1H	HOH	8	8.399	18.988	22.917	1.00	0.00	H
HETATM	761	2H	HOH	8	9.047	20.193	23.630	1.00	0.00	H
HETATM	762	O	HOH	9	14.426	18.177	16.971	1.00	91.64	O
HETATM	763	1H	HOH	9	15.010	18.890	16.831	1.00	0.00	H
HETATM	764	2H	HOH	9	13.573	18.570	17.105	1.00	0.00	H
HETATM	765	O	HOH	10	6.660	18.291	14.901	1.00	47.78	O
HETATM	766	1H	HOH	10	6.912	18.615	14.042	1.00	0.00	H
HETATM	767	2H	HOH	10	7.036	18.893	15.527	1.00	0.00	H
HETATM	768	O	HOH	11	9.801	17.869	7.746	1.00	50.95	O
HETATM	769	1H	HOH	11	9.411	16.994	7.627	1.00	0.00	H
HETATM	770	2H	HOH	11	10.574	17.739	8.259	1.00	0.00	H
HETATM	771	O	HOH	12	7.790	15.753	8.005	1.00	53.41	O
HETATM	772	1H	HOH	12	7.613	15.541	8.927	1.00	0.00	H
HETATM	773	2H	HOH	12	8.562	15.235	7.778	1.00	0.00	H
HETATM	774	O	HOH	13	14.145	18.206	2.097	1.00	57.88	O
HETATM	775	1H	HOH	13	14.620	17.400	2.308	1.00	0.00	H
HETATM	776	2H	HOH	13	13.290	18.116	2.522	1.00	0.00	H
HETATM	777	O	HOH	14	12.314	6.447	-8.867	1.00	65.60	O
HETATM	778	1H	HOH	14	12.737	7.223	-9.273	1.00	0.00	H
HETATM	779	2H	HOH	14	12.746	6.378	-8.026	1.00	0.00	H
HETATM	780	O	HOH	15	21.545	-1.804	-13.790	1.00	49.07	O
HETATM	781	1H	HOH	15	21.496	-2.647	-14.243	1.00	0.00	H
HETATM	782	2H	HOH	15	20.714	-1.364	-13.979	1.00	0.00	H
HETATM	783	O	HOH	16	22.569	8.158	-11.409	1.00	46.71	O
HETATM	784	1H	HOH	16	22.403	7.556	-10.690	1.00	0.00	H
HETATM	785	2H	HOH	16	22.970	8.920	-10.966	1.00	0.00	H
HETATM	786	O	HOH	17	15.788	9.728	-7.160	1.00	65.57	O
HETATM	787	1H	HOH	17	16.729	9.881	-7.059	1.00	0.00	H
HETATM	788	2H	HOH	17	15.600	8.894	-6.726	1.00	0.00	H
HETATM	789	O	HOH	18	7.205	11.385	12.307	1.00	55.74	O
HETATM	790	1H	HOH	18	8.081	11.402	11.900	1.00	0.00	H
HETATM	791	2H	HOH	18	6.937	12.318	12.282	1.00	0.00	H
HETATM	792	O	HOH	19	9.847	10.295	-2.390	1.00	38.62	O
HETATM	793	1H	HOH	19	8.917	10.375	-2.193	1.00	0.00	H
HETATM	794	2H	HOH	19	10.216	9.724	-1.732	1.00	0.00	H
HETATM	795	O	HOH	20	14.009	23.313	28.896	1.00	73.77	O
HETATM	796	1H	HOH	20	14.838	23.163	28.435	1.00	0.00	H
HETATM	797	2H	HOH	20	13.892	22.574	29.472	1.00	0.00	H
HETATM	798	O	HOH	21	13.472	10.407	-8.621	1.00	45.61	O
HETATM	799	1H	HOH	21	13.745	10.082	-9.473	1.00	0.00	H
HETATM	800	2H	HOH	21	14.142	10.063	-8.014	1.00	0.00	H
HETATM	801	O	HOH	22	11.244	11.155	-10.623	1.00	56.60	O
HETATM	802	1H	HOH	22	10.350	11.480	-10.481	1.00	0.00	H
HETATM	803	2H	HOH	22	11.708	11.979	-10.633	1.00	0.00	H
HETATM	804	O	HOH	23	4.167	17.232	14.430	1.00	59.26	O
HETATM	805	1H	HOH	23	3.234	17.266	14.255	1.00	0.00	H

FIG. 5N

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HETATM  806  2H   HOH    23       4.325  17.835  15.160  1.00  0.00           H
HETATM  807   O   HOH    24       7.289  13.019   7.362  1.00 59.36           O
HETATM  808  1H   HOH    24       6.985  13.870   7.006  1.00  0.00           H
HETATM  809  2H   HOH    24       6.571  12.413   7.174  1.00  0.00           H
HETATM  810   O   HOH    25       7.898  10.616   4.187  1.00 53.34           O
HETATM  811  1H   HOH    25       8.656  10.430   4.750  1.00  0.00           H
HETATM  812  2H   HOH    25       8.245  10.424   3.311  1.00  0.00           H
HETATM  813   O   HOH    26      18.700   5.086   6.487  1.00 58.77           O
HETATM  814  1H   HOH    26      19.339   4.385   6.621  1.00  0.00           H
HETATM  815  2H   HOH    26      18.262   5.154   7.320  1.00  0.00           H
HETATM  816   O   HOH    27      14.706   8.287 -15.323  1.00 71.36           O
HETATM  817  1H   HOH    27      13.983   8.106 -15.937  1.00  0.00           H
HETATM  818  2H   HOH    27      15.493   8.205 -15.863  1.00  0.00           H
HETATM  819   O   HOH    28      17.583  10.761 -18.187  1.00 49.62           O
HETATM  820  1H   HOH    28      17.448  10.166 -18.942  1.00  0.00           H
HETATM  821  2H   HOH    28      17.684  10.091 -17.473  1.00  0.00           H
HETATM  822   O   HOH    29      16.849  14.385 -20.221  1.00 59.72           O
HETATM  823  1H   HOH    29      16.623  13.960 -19.443  1.00  0.00           H
HETATM  824  2H   HOH    29      16.025  14.098 -20.716  1.00  0.00           H
HETATM  825   O   HOH    30      23.359  25.370  14.837  1.00 57.74           O
HETATM  826  1H   HOH    30      23.884  26.063  14.430  1.00  0.00           H
HETATM  827  2H   HOH    30      23.387  25.608  15.758  1.00  0.00           H
HETATM  828   O   HOH    31      17.498  22.874  16.925  1.00 93.45           O
HETATM  829  1H   HOH    31      17.242  23.753  16.701  1.00  0.00           H
HETATM  830  2H   HOH    31      16.839  22.592  17.567  1.00  0.00           H
HETATM  831   O   HOH    32      20.348  23.693  23.117  1.00 63.40           O
HETATM  832  1H   HOH    32      21.038  23.780  23.785  1.00  0.00           H
HETATM  833  2H   HOH    32      20.407  22.764  22.840  1.00  0.00           H
HETATM  834   O   HOH    33      26.302  25.733  28.760  1.00 74.83           O
HETATM  835  1H   HOH    33      26.307  26.586  28.361  1.00  0.00           H
HETATM  836  2H   HOH    33      25.982  25.835  29.661  1.00  0.00           H
HETATM  837   O   HOH    34      25.950  24.779  25.047  1.00 73.62           O
HETATM  838  1H   HOH    34      26.734  24.588  25.612  1.00  0.00           H
HETATM  839  2H   HOH    34      26.332  25.366  24.401  1.00  0.00           H
HETATM  840   O   HOH    35      11.696  17.842   0.575  1.00 63.54           O
HETATM  841  1H   HOH    35      12.559  17.505   0.750  1.00  0.00           H
HETATM  842  2H   HOH    35      11.078  17.126   0.562  1.00  0.00           H
HETATM  843   O   HOH    36      14.262  19.203   4.844  1.00 48.44           O
HETATM  844  1H   HOH    36      13.591  19.435   5.469  1.00  0.00           H
HETATM  845  2H   HOH    36      15.124  19.290   5.226  1.00  0.00           H
HETATM  846   O   HOH    37      15.984  22.052  -2.490  1.00 62.80           O
HETATM  847  1H   HOH    37      15.327  21.946  -3.200  1.00  0.00           H
HETATM  848  2H   HOH    37      15.529  21.751  -1.706  1.00  0.00           H
HETATM  849   O   HOH    38      16.135  20.908  -5.213  1.00 82.35           O
HETATM  850  1H   HOH    38      16.482  20.062  -4.835  1.00  0.00           H
HETATM  851  2H   HOH    38      15.378  20.538  -5.665  1.00  0.00           H
HETATM  852   O   HOH    39      10.937   6.573  -6.161  1.00 63.06           O
HETATM  853  1H   HOH    39      11.244   5.996  -5.478  1.00  0.00           H
HETATM  854  2H   HOH    39      11.691   7.003  -6.564  1.00  0.00           H
HETATM  855   O   HOH    40       9.077  12.911  -2.911  1.00 64.88           O
HETATM  856  1H   HOH    40       8.184  13.199  -3.064  1.00  0.00           H
HETATM  857  2H   HOH    40       9.394  12.597  -3.765  1.00  0.00           H
HETATM  858   O   HOH    41      13.272   7.391  13.889  1.00 65.83           O
HETATM  859  1H   HOH    41      13.766   6.842  13.286  1.00  0.00           H
HETATM  860  2H   HOH    41      13.421   8.306  13.606  1.00  0.00           H
HETATM  861   O   HOH    42       6.871  10.837  16.390  1.00 58.39           O
HETATM  862  1H   HOH    42       6.258  11.055  15.679  1.00  0.00           H
HETATM  863  2H   HOH    42       7.611  11.410  16.223  1.00  0.00           H
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FIG. 50

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HETATM  864   O   HOH     43      14.184  12.148  23.463  1.00 73.66           O
HETATM  865 1H   HOH     43      14.543  11.552  22.797  1.00  0.00           H
HETATM  866 2H   HOH     43      13.316  12.368  23.168  1.00  0.00           H
END
```

FIG. 5P

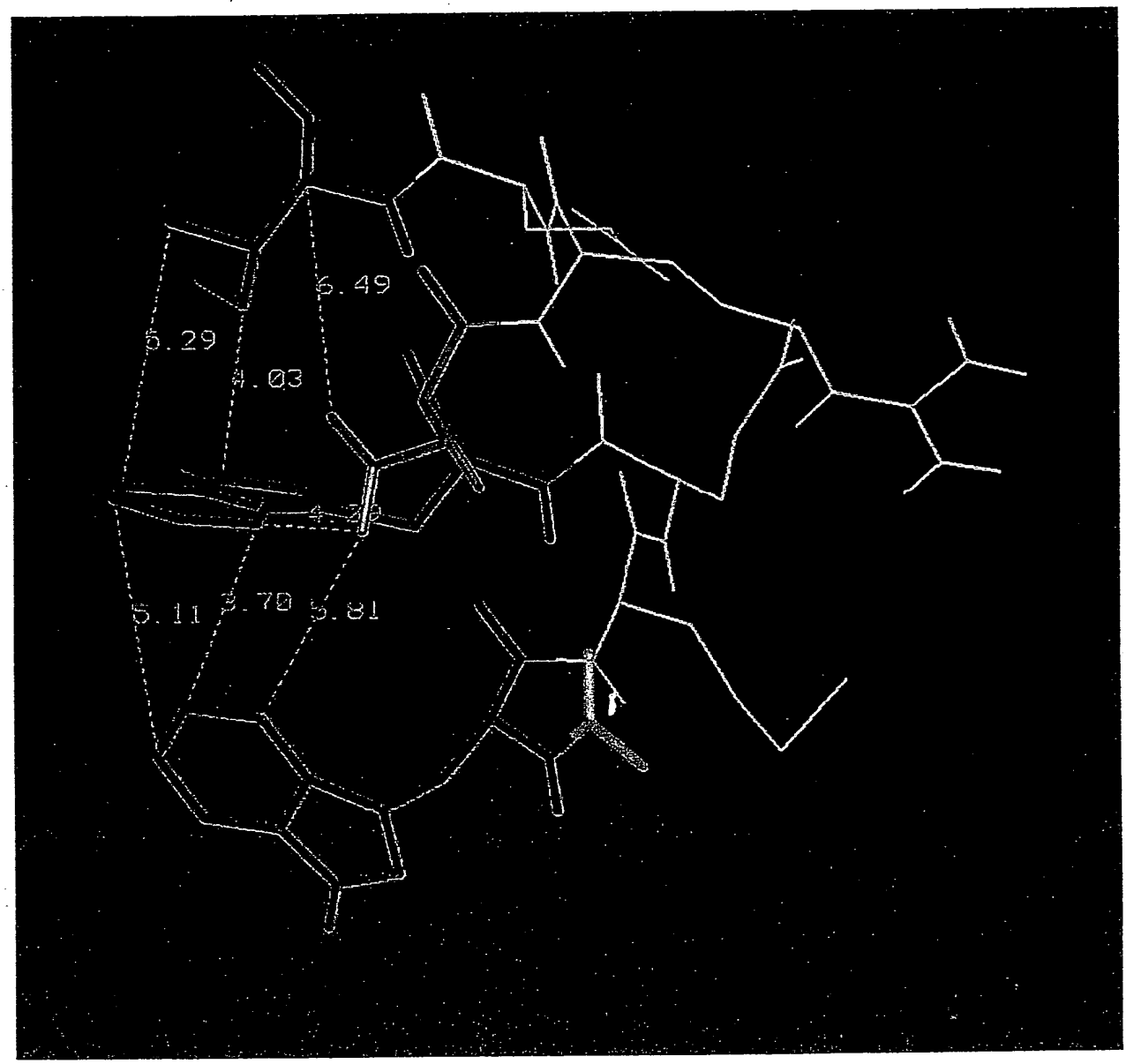

FIG. 6

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